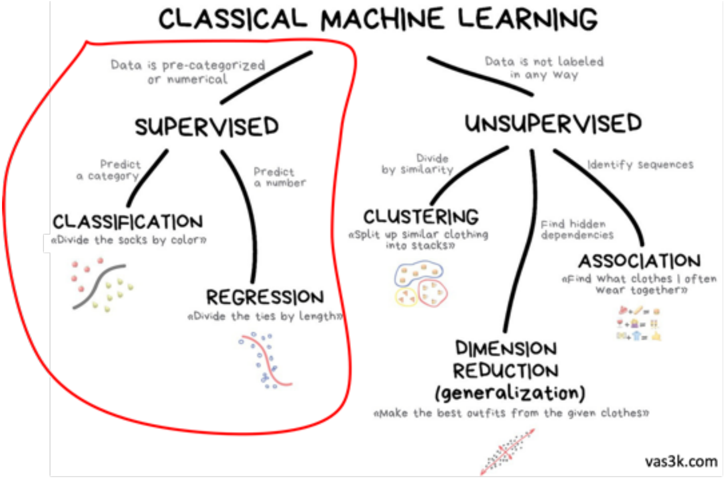
Learning with Linear Models: Foundations of Machine Learning

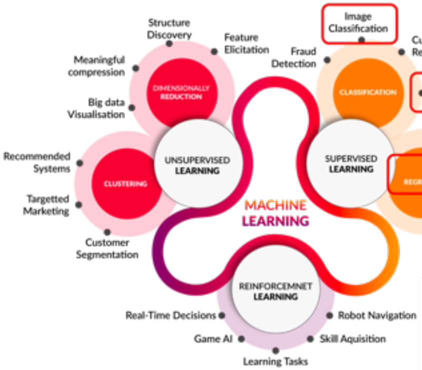
Mário A. T. Figueiredo

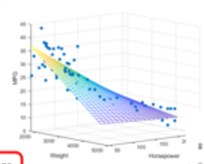
14th Lisbon Machine Learning School, July 11, 2024

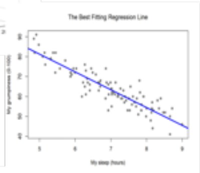

CLASSICAL MACHINE LEARNING
Data is pre-categorized or numerical
Data is not labeled in any way
SUPERVISED
UNSUPERVISED
Predict a category
Predict a number
CLASSIFICATION
«Divide the socks by color»
REGRESSION
«Divide the ties by length»
Divide by similarity
Identify sequences
CLUSTERING
«Split up similar clothing into stacks»
Find hidden dependencies
ASSOCIATION
«Find what clothes I often wear together»
DIMENSION REDUCTION (generalization)
«Make the best outfits from the given clothes»
vas3k.com

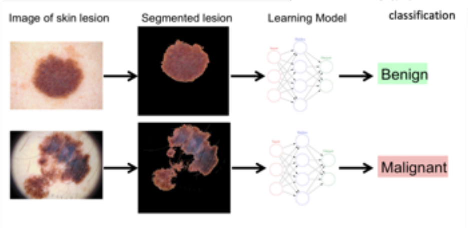
Supervised Learning

Types od Machine Learning









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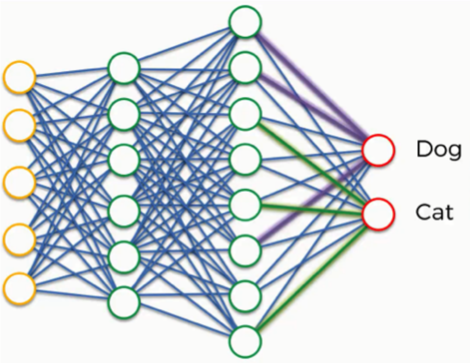
  - ✓ Linear models are a component of deep networks.
  - ✓ It is the natural starting point to start learning machine learning.

Linear Classifiers and Neural Networks



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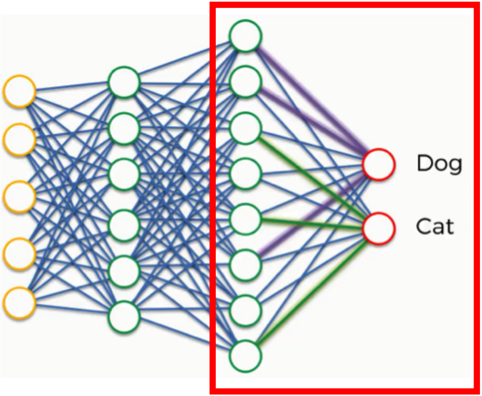

Linear Classifier

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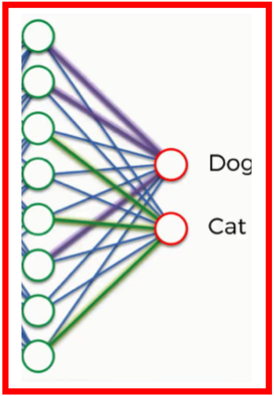

Linear Classifier

Outline

1. Introduction
2. Regression
3. Classification
4. Optimization for Supervised Learning

Supervised Machine Learning

- Given a collection of input/output pairs (training data)

$$\mathcal{D} = (\boldsymbol{x}_1, y_1), ..., (\boldsymbol{x}_N, y_N) \in \mathcal{X} \times \mathcal{Y} \qquad (\boldsymbol{x}_i \in \mathcal{X},\ y_i \in \mathcal{Y})$$

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- Hopefully, $\widehat{y} \approx y$ most of the time, i.e., h should **generalize**.

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  - ✓ e.g., a **news article** together with a **topic**
  - ✓ e.g., a **sentence** together with its **translation**
  - ✓ e.g., a **sequence of words (tokens)** together with the **next word**
  - ✓ e.g., an **image** partitioned into **segmentation regions**

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- **Structured classification:** $\mathcal{Y}$ exponentially large and structured
  - ✓ e.g., machine translation, caption generation, image segmentation, ...

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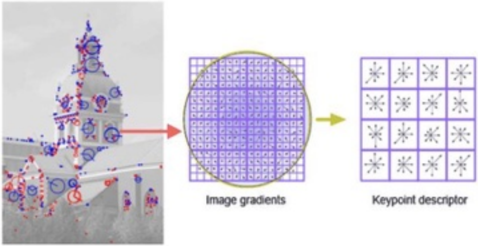

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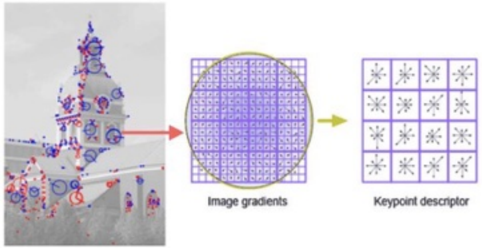

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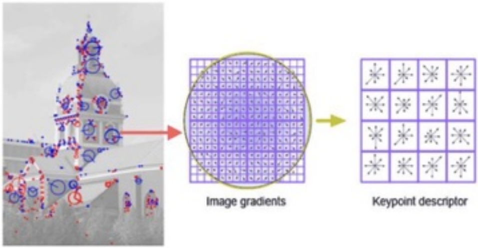

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  - ✓ Decades of research in machine learning, natural language processing, computer vision, image analysis, speech processing, ...

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- Categorical features are often reduced to one-hot binary features:

$$\boldsymbol{e}_y := (0, \ldots, 0, \underbrace{1}_{\text{position } y}, 0, \ldots, 0) \in \{0,\, 1\}^K \text{ represents class } y$$

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Tomorrow's lecture, by Bhiksha Raj

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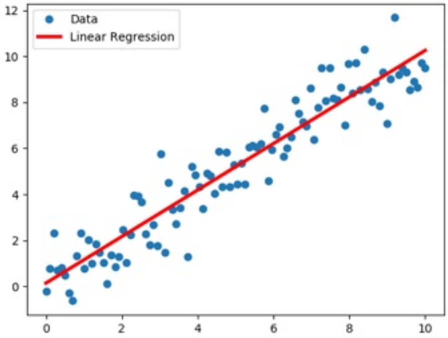

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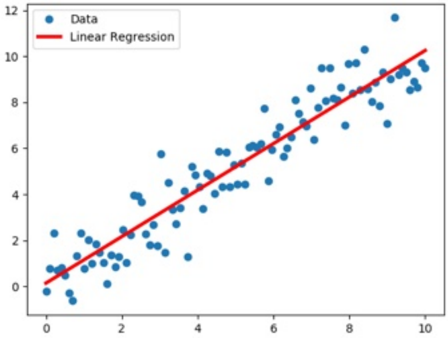

"When you're fundraising, it's AI.

When you're hiring, it's ML.

When you're implementing, it's just linear regression"

(Baron Schwartz)

Linear (Nonlinear) Regression

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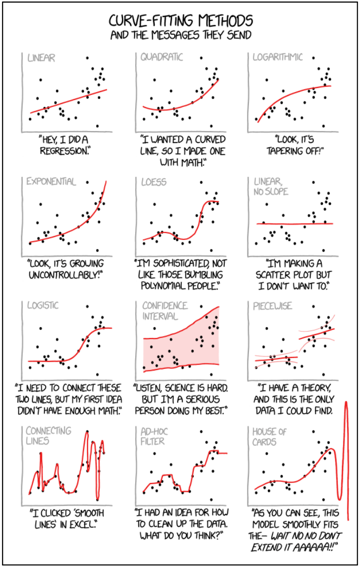
  (more later)



xkcd.com

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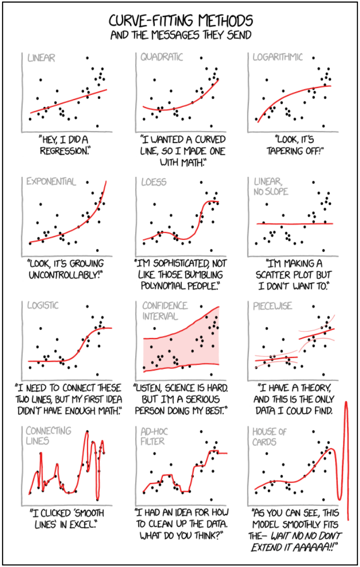
- Beware the inductive bias



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Regression

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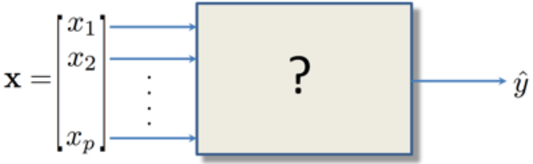

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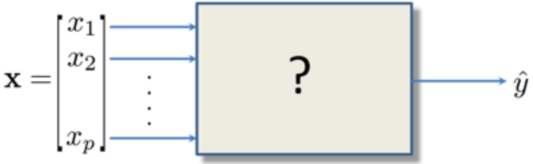

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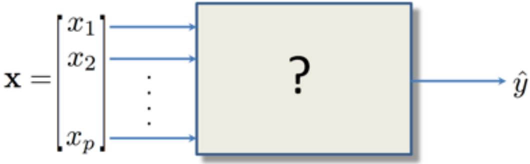

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- Notation: **bold** = vector or matrix (e.g. $\boldsymbol{x}$, $\boldsymbol{X}$).

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- Likelihood and log-likelihood function

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$$\log f_{Y_1,...,Y_n}(y_1, ..., y_n|\boldsymbol{x}_1, ..., \boldsymbol{x}_n, \boldsymbol{w}, w_0, \sigma^2) = K - \frac{1}{2\sigma^2} \sum_{i=1}^{n} (y_i - \boldsymbol{w}^T \boldsymbol{x}_i - w_0)^2$$

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- Maximum likelihood estimate of $\mathbf{w}$:

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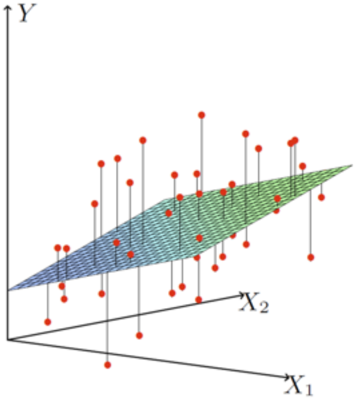
$$(\hat{\boldsymbol{w}}, \hat{w}_0)_{\mathsf{ERM}} = (\hat{\boldsymbol{w}}, \hat{w}_0)_{\mathsf{LS}} = \arg\min_{\boldsymbol{w}, w_0} R_{\mathsf{emp}}[\boldsymbol{w}, w_0]$$

Linear Regression: Another Picture



Linear least squares fitting with $X \in \mathbb{R}^2$. We seek the linear function of X that minimizes the sum of squared residuals from Y.

From: Hastie, Tibshirani, Friedman, "The Elements of Statistical Learning", Springer, 2009.

Linear Regression: Dealing with w_0 (1st Method)

- Replace each original $\boldsymbol{x}_i$ with $\boldsymbol{x}_i = \begin{bmatrix} 1 \\ x_{i1} \\ \vdots \\ x_{ip} \end{bmatrix} \in \mathbb{R}^{p+1}$

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- The offset w_0 is now absorbed into $\boldsymbol{w}^T\boldsymbol{x}_i$, thus

$$\hat{\boldsymbol{w}}_{\mathsf{LS}} = \arg\min_{\boldsymbol{w}} \sum_{i=1}^{n} (y_i - \boldsymbol{w}^T\boldsymbol{x}_i)^2$$

Linear Regression: Dealing with w_0 (2nd Method)

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...which we will assume hereafter to be true.

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...only if $\boldsymbol{X}^T\boldsymbol{X}$ is invertible, *i.e.*, $\texttt{rank}(\boldsymbol{X}) = p$, requiring $n \geq p$.

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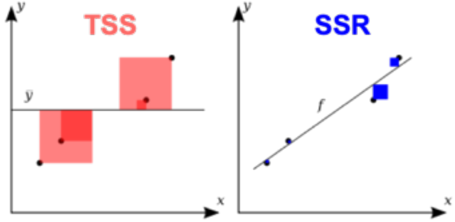

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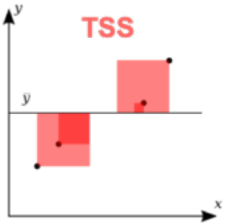

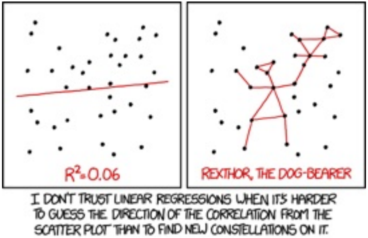

The Geometry of Linear Regression

- Predicted values at the sampled points:

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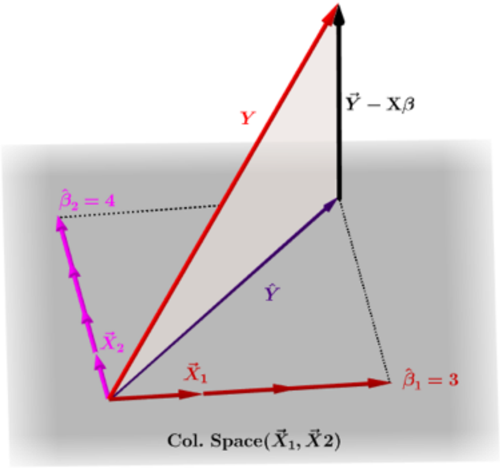
i.e., the orthogonal projection onto $\operatorname{range}(\boldsymbol{X})$.

Geometry of Linear Regression: Euclidean Projection

This picture is in $\mathbb{R}^n$



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$$\boldsymbol{\phi} : \mathbb{R}^p \rightarrow \mathbb{R}^d, \quad \boldsymbol{\phi}(\boldsymbol{x}) = \begin{bmatrix} \phi_0(\boldsymbol{x}) \\ \vdots \\ \phi_{d-1}(\boldsymbol{x}) \end{bmatrix} \quad \text{(typically } \phi_0(\boldsymbol{x}) = 1\text{)}$$

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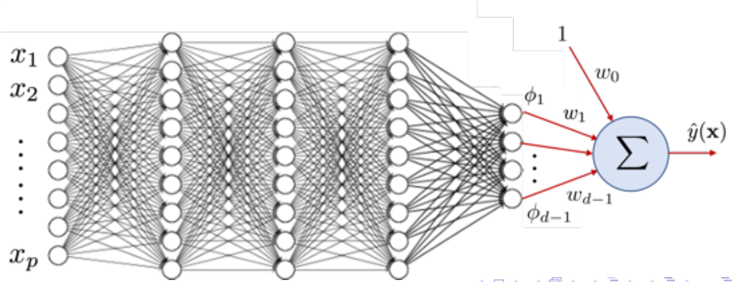
- E.g., final layer of a deep network:



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- The LS criterion becomes

$$\begin{aligned} \hat{\boldsymbol{w}}_{\text{LS}} &= \arg\min_{\boldsymbol{w}} \sum_{i=1}^{n} (y_i - \boldsymbol{w}^T \boldsymbol{\phi}(\boldsymbol{x}_i))^2 \\ &= \arg\min_{\boldsymbol{w}} \|\boldsymbol{y} - \boldsymbol{X}\boldsymbol{w}\|_2^2, \end{aligned}$$

where the design matrix $\boldsymbol{X}$ is now

$$\boldsymbol{X} = \begin{bmatrix} \phi_0(\boldsymbol{x}_1) & \cdots & \phi_{d-1}(\boldsymbol{x}_1) \\ \vdots & \ddots & \vdots \\ \phi_0(\boldsymbol{x}_n) & \cdots & \phi_{d-1}(\boldsymbol{x}_n) \end{bmatrix} \in \mathbb{R}^{n \times (d)}$$

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...all monomials of order up to k

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Example: Polynomial Regression

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- which has dimension

$$d = \binom{p+k}{k} = \frac{(p+k)!}{k!\,p!} \geq \left(\frac{p+k}{k}\right)^k$$

...exponential in k

Other Types of Non-Linear Regression

- Radial basis functions (RBF): $\phi_j(\boldsymbol{x}) = \psi\Big(\dfrac{1}{\alpha_j}\|\boldsymbol{x} - \boldsymbol{c}_j\|_2\Big)$

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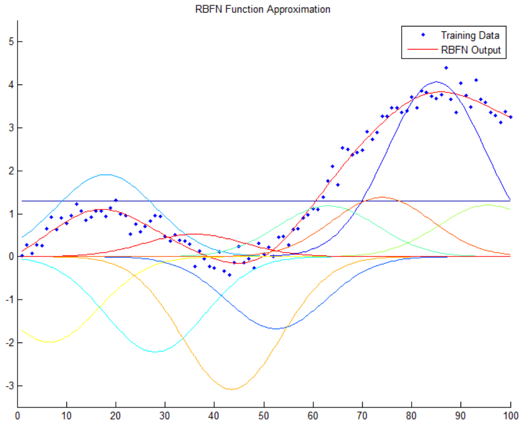
- Kernels: more later.

Example of Gaussian RBF Regression



Ridge Regression

- If $\mathtt{rank}(\boldsymbol{X}) < p$ (for example, if $n < p$), $\hat{\boldsymbol{w}}_{\mathsf{LS}}$ cannot be computed,

  $(\boldsymbol{X}^T\boldsymbol{X}) \in \mathbb{R}^{p\times p}; \quad \mathtt{rank}(\boldsymbol{X}) < p \;\Rightarrow\; (\boldsymbol{X}^T\boldsymbol{X})^{-1}$ cannot be computed

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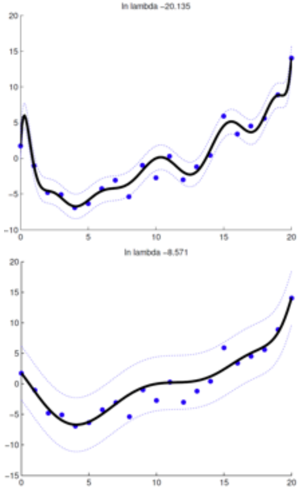
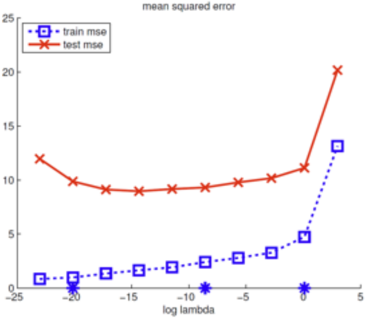
- Goes by other names in other contexts: *weight decay, penalized least squares, Tikhonov regularization,* ℓ_2 regularization,...

Ridge Regression: Illustration

Even if $\hat{\boldsymbol{w}}_{\text{LS}}$ can be computed, $\hat{\boldsymbol{w}}_{\text{ridge}}$ may preferable (lower MSE)

Example: fitting an order-14 polynomial to 21 points in $\mathbb{R}$





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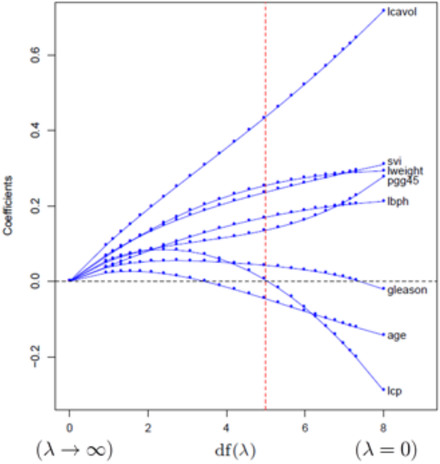
- Example with $p = 8$ (prostate cancer data; Hastie at al, 2009)



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- Extreme case: $K = n$, leave-one-out CV (LOOCV).

Dual Variables: Ridge Regression

- Ridge regression: $\hat{\boldsymbol{w}}_{\text{ridge}}(\boldsymbol{y})$ is the solution w.r.t. $\boldsymbol{w}$ of

$$\big(\boldsymbol{X}^T\boldsymbol{X} + \lambda\boldsymbol{I}\big)\boldsymbol{w} = \boldsymbol{X}^T\boldsymbol{y} \quad \Leftrightarrow \quad \hat{\boldsymbol{w}}_{\text{ridge}}(\boldsymbol{y}) = \frac{1}{\lambda}\boldsymbol{X}^T\big(\boldsymbol{y} - \boldsymbol{X}\,\hat{\boldsymbol{w}}_{\text{ridge}}(\boldsymbol{y})\big)$$

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$$\hat{y}(\boldsymbol{x}) = \boldsymbol{x}^T\hat{\boldsymbol{w}}_{\text{ridge}}(\boldsymbol{y}) = \sum_{i=1}^{n}\alpha_i\left(\boldsymbol{x}^T\boldsymbol{x}_i\right)$$

...a linear combination of the inner products of $\boldsymbol{x}$ with the $\boldsymbol{x}_i$

Dual Variables: Ridge Regression (2)

- Ridge regression in dual variables:

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Kernel Regression

- Recall that, in dual variables,

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- The feature map moves the inner products from $\mathbb{R}^p$ to $\mathbb{R}^d$. Bad?

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- Motivation example: order 2 polynomial regression in $\mathbb{R}^2$:

$$\phi(\boldsymbol{x}) = \phi([x_1,\, x_2]^T) = [1, {x_1}^2, {x_2}^2, \sqrt{2}\, x_1\, x_2]$$

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$$\langle \phi(\boldsymbol{x}), \phi(\boldsymbol{x}') \rangle = 1 + {x_1}^2\, {x_1'}^2 + {x_2}^2\, {x_2'}^2 + 2\, x_1\, x_1'\, x_2\, x_2' = 1 + \langle \boldsymbol{x}, \boldsymbol{x}' \rangle^2$$

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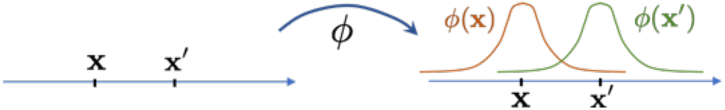

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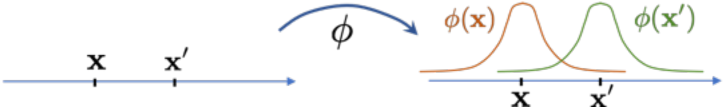

- Why?

$$\langle \boldsymbol{\phi}(\boldsymbol{x}), \boldsymbol{\phi}(\boldsymbol{x}') \rangle = \int \exp\left(-\frac{\|\boldsymbol{x} - \boldsymbol{u}\|_2^2}{2\sigma^2}\right) \exp\left(-\frac{\|\boldsymbol{x}' - \boldsymbol{u}\|_2^2}{2\sigma^2}\right) d\boldsymbol{u} = \exp\left(-\frac{\|\boldsymbol{x} - \boldsymbol{x}'\|_2^2}{2\sigma^2}\right)$$

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Double Descent

Reconciling modern machine-learning practice and the classical bias–variance trade-off

Mikhail Belkin[a,b,1], Daniel Hsu[c], Siyuan Ma[a], and Soumik Mandal[a]

[a]Department of Computer Science and Engineering, The Ohio State University, Columbus, OH 43210; [b]Department of Statistics, The Ohio State University, Columbus, OH 43210; and [c]Computer Science Department and Data Science Institute, Columbia University, New York, NY 10027

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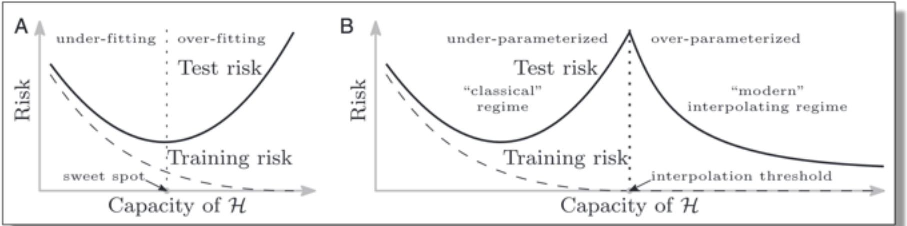
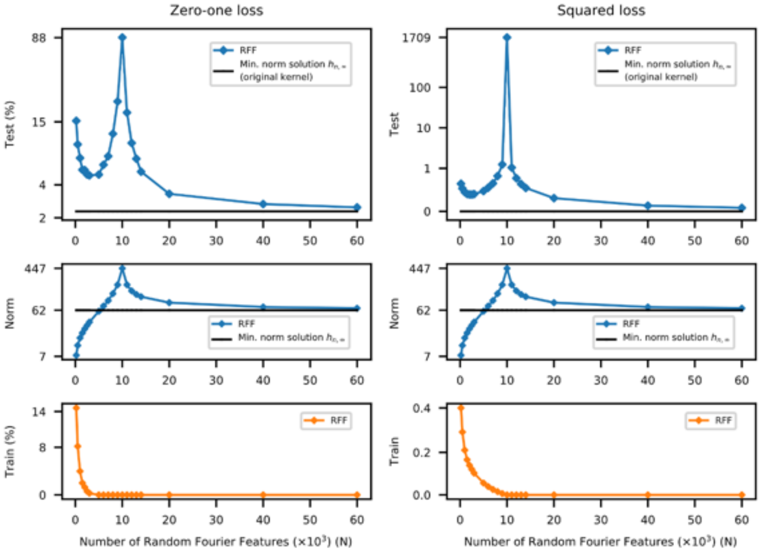


Double Descent (2)

- Random Fourier features: $\phi_i(\boldsymbol{x}) = \exp(\sqrt{-1}\langle \boldsymbol{v}_i, \boldsymbol{x}\rangle), \;\; \boldsymbol{v}_i \sim \mathcal{N}(0, \boldsymbol{I})$



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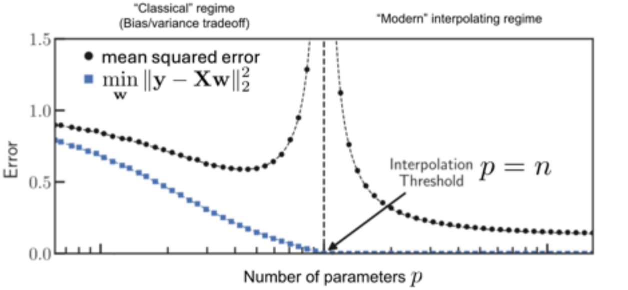

(Image adapted from Rocks and Mehta, 2022.)

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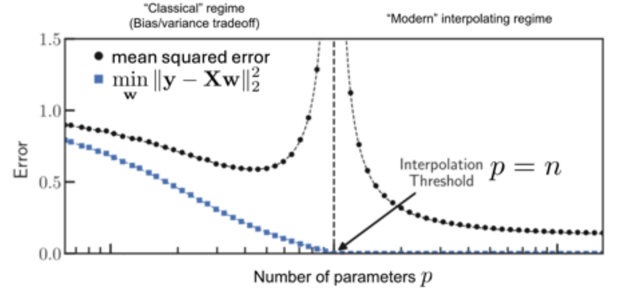

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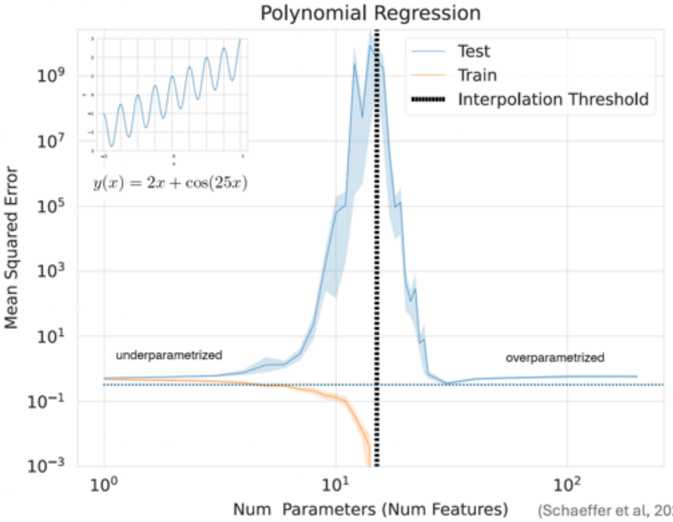
- Current research topic.

Overparametrization and Double Descent (cont.)

- Polynomial regression: the ϕ_i are Legendre polynomials.



(Schaeffer et al, 2023)

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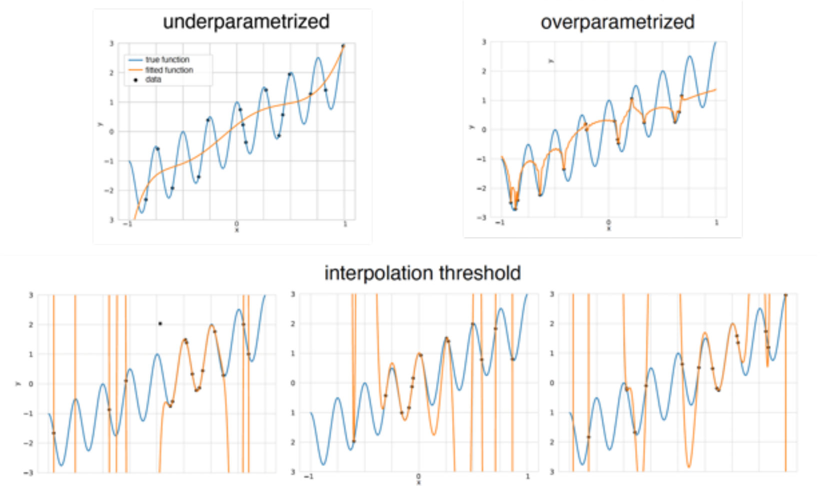

Bayesian View of Ridge Regression

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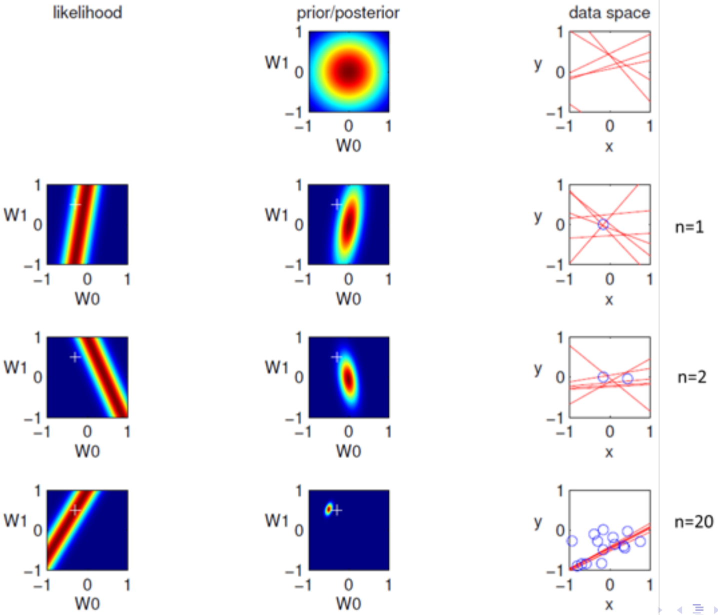
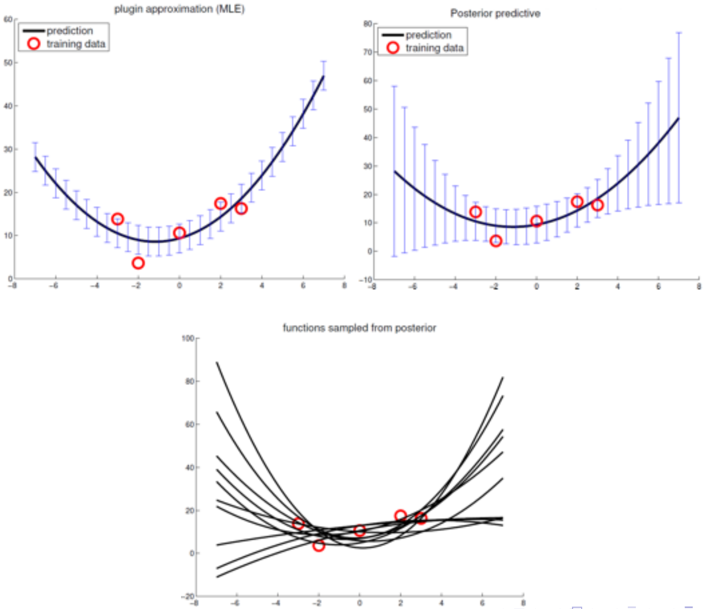
- Example in next slide: $p = 1$, $\boldsymbol{w} = [w_0,\, w_1]^T$, $\boldsymbol{w}_{\text{true}} = [-0.3,\, 0.5]$

Bayesian View of Ridge Regression: Example 1



Bayesian View of Ridge Regression: Example 2



Gaussian Processes

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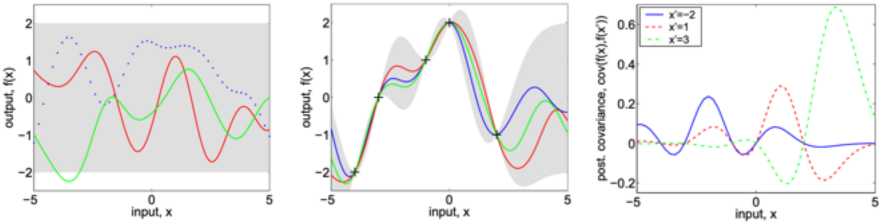
- Posterior: $\boldsymbol{F}' | (\boldsymbol{F} = \boldsymbol{f}) \sim$

$$\mathcal{N}\left(K(\boldsymbol{X}', \boldsymbol{X})\, K(\boldsymbol{X}, \boldsymbol{X})^{-1} \boldsymbol{f}, K(\boldsymbol{X}', \boldsymbol{X}') - K(\boldsymbol{X}', \boldsymbol{X}) K(\boldsymbol{X}, \boldsymbol{X})^{-1} K(\boldsymbol{X}, \boldsymbol{X}')\right)$$

Gaussian Process Example: Noiseless Observations (2)

- Left: samples from the "prior" $\boldsymbol{F}$;
- Middle: samples from "posterior" $\boldsymbol{F}'|\boldsymbol{F} = \boldsymbol{f}$ (crosses);
- Gray bands: 95% probability.
- Right: posterior covariance



(a), prior (b), posterior (c), posterior covariance

(figure from Rasmussen & Williams, 2006)

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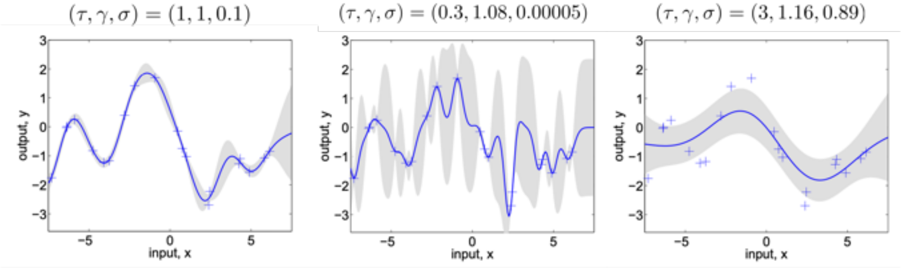
- Letting $\boldsymbol{\alpha} = \left(K(\boldsymbol{X}, \boldsymbol{X}) + \sigma^2 \boldsymbol{I}\right)^{-1} \boldsymbol{y}$, then $\hat{\boldsymbol{f}} = K(\boldsymbol{X}', \boldsymbol{X})\, \boldsymbol{\alpha}$, and

$$\hat{f}(\boldsymbol{x}'_i) = \sum_{j=1}^{n} \alpha_j K(\boldsymbol{x}'_i, \boldsymbol{x}_j)$$

...GP regression is kernel regression.

Gaussian Process Regression: Example

- Gaussian RBF kernel: $K(\boldsymbol{x}, \boldsymbol{x}') = \gamma^2 \exp\left(-\frac{\|\boldsymbol{x}-\boldsymbol{x}'\|_2^2}{2\,\tau^2}\right)$
- τ controls the correlation length-scale; γ^2 is the point-wise variance.
- Left: 20 samples with $(\tau, \gamma, \sigma) = (1, 1, 0.1)$; middle and right: GP regressions with different parameters.



(figure from Rasmussen & Williams, 2006)

LASSO regression

- Alternative to ridge regression, with built-in variable selection

$$\hat{\boldsymbol{w}}_{\text{lasso}} = \arg\min_{\boldsymbol{w}} \; \frac{1}{2}\|\boldsymbol{y} - \boldsymbol{X}\boldsymbol{w}\|_2^2 + \lambda\,\|\boldsymbol{w}\|_1$$

  where $\|\boldsymbol{w}\|_1 = \sum_i |w_i|$, the ℓ_1 norm.

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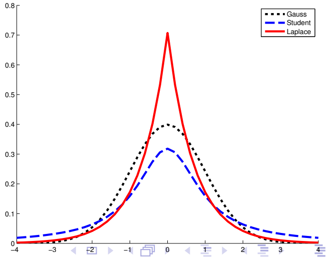
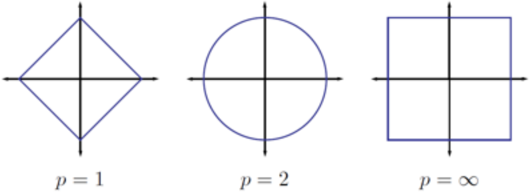
- Can be seen as MAP estimate of $\boldsymbol{w}$, under Laplacian prior

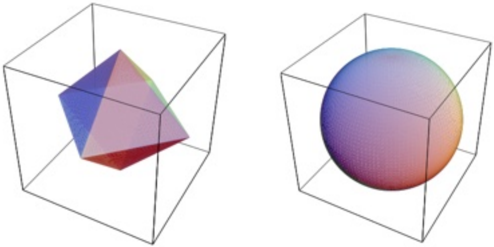
$$f_{\boldsymbol{W}}(\boldsymbol{w}) = \prod_{i=1}^{p} \frac{\lambda}{2} \exp\Big(-\lambda|w_i|\Big) = \left(\frac{\lambda}{2}\right)^p \exp\Big(-\lambda\|\boldsymbol{w}\|_1\Big)$$



Norm balls

Radius r ball in ℓ_p norm: $\quad B_p(r) = \{\boldsymbol{v} \in \mathbb{R}^n : \|\boldsymbol{v}\|_p \leq r\}$





$p = 1$ $\qquad\qquad$ $p = 2$

Why LASSO Yields Sparse Solutions?

- $\displaystyle \min_{\boldsymbol{w}} \frac{1}{2}\|\boldsymbol{y} - \boldsymbol{X}\boldsymbol{w}\|_2^2 + \lambda \|\boldsymbol{w}\|$ and $\displaystyle \min_{\boldsymbol{w}} \|\boldsymbol{y} - \boldsymbol{X}\boldsymbol{w}\|_2^2$ s.t. $\|\boldsymbol{w}\| \leq \delta$

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- Ridge ($\|\boldsymbol{w}\|_2$) versus LASSO ($\|\boldsymbol{w}\|_1$)

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Why LASSO Yields Sparse Solutions?

- $\min_{\boldsymbol{w}} \frac{1}{2}\|\boldsymbol{y} - \boldsymbol{X}\boldsymbol{w}\|_2^2 + \lambda\,\|\boldsymbol{w}\|$ and $\min_{\boldsymbol{w}} \|\boldsymbol{y} - \boldsymbol{X}\boldsymbol{w}\|_2^2$ s.t. $\|\boldsymbol{w}\| \leq \delta$

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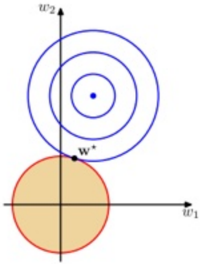

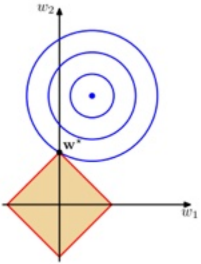

LASSO Yields Sparse Solutions

- The simplest problem with ℓ_1 regularization ($p = 1$)

$$\widehat{w} = \arg\min_w \frac{1}{2}(w-y)^2 + \lambda|w| = \mathsf{soft}(y,\lambda) = \begin{cases} y-\lambda & \Leftarrow & y > \lambda \\ 0 & \Leftarrow & |y| \leq \lambda \\ y+\lambda & \Leftarrow & y < -\lambda \end{cases}$$

$$\begin{aligned} \mathsf{soft}(y,\lambda) &= \mathsf{sign}(y)\big(|y| - \lambda\big)_+ \\ &= \mathsf{sign}(y)\max\big(|y| - \lambda, 0\big) \end{aligned}$$

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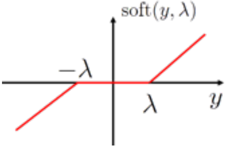

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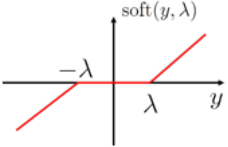

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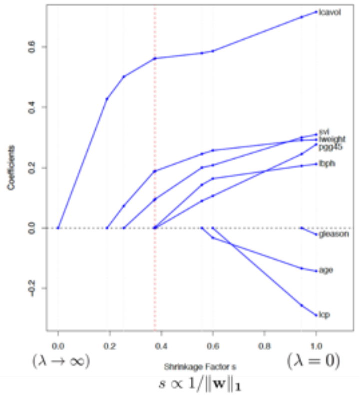
- Contrast with the squared ℓ_2 (ridge) regularizer (linear scaling):

$$\widehat{w} = \arg\min_w \frac{1}{2}(w-y)^2 + \frac{\lambda}{2}\,w^2 = \frac{1}{1+\lambda}\,y$$

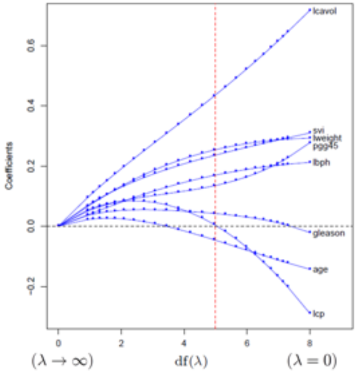
LASSO versus Ridge

- Example (prostate cancer data)

LASSO



Ridge



Solving LASSO Regression

- Ridge regression simply amounts to solving a linear system:

$$(\boldsymbol{X}^T\boldsymbol{X} + \lambda\boldsymbol{I})\hat{\boldsymbol{w}}_{\text{ridge}} = \boldsymbol{X}^T\boldsymbol{y}$$

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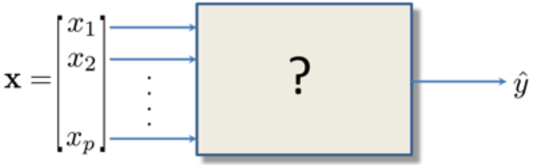
- In deep learning, with gradient descent, simply pretend that ℓ_1 is differentiable (derivative in $\{-1, 0, 1\}$), although it is crucial to adapt the step size.

Outline

1. Introduction
2. Regression
3. **Classification**
4. Optimization for Supervised Learning

Classification (a.k.a. Pattern Recognition)

- In a nutshell: produce a "machine" that predicts/estimates/guesses a class $y \in \{1, ..., K\}$, from variables/features x_1,...,x_p



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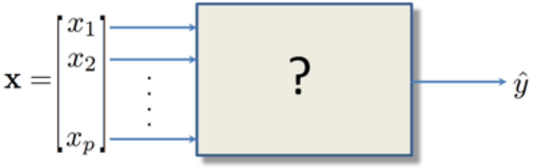

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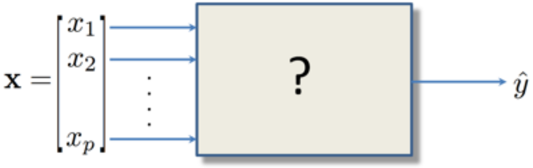

- Maybe the core machine learning problem, with countless applications.
- Learning/training: given a collection of examples (training data)

$$\mathcal{D} = \big((\mathbf{x}_1, y_1), ..., (\mathbf{x}_n, y_n)\big)$$

..find the "best" possible machine.

Generative Perspective: Exponential Family Classes

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- Examples: Gaussian, Exponential, Binomial, Multinomial, Poisson, ...

Class Posteriors for Exponential Family Classes

- Class posterior probabilities (from Bayes law):

$$
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f_{Y|\boldsymbol{X}}(y|\boldsymbol{x}) &\propto f_Y(y)\, f_{\boldsymbol{X}|Y}(\boldsymbol{x}|y)\\
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- Normalizing,

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f_{Y|\boldsymbol{X}}(y|\boldsymbol{x}) = \frac{\exp\Big((\boldsymbol{\eta}^{(y)})^T\boldsymbol{\phi}(\boldsymbol{x}) + \zeta^{(y)}\Big)}{\displaystyle\sum_{u=1}^{K}\exp\Big((\boldsymbol{\eta}^{(u)})^T\boldsymbol{\phi}(\boldsymbol{x}) + \zeta^{(u)}\Big)}
$$

...sometimes called a generalized linear model (GLM) or softmax.

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- Plug these estimates in the MAP classifier of the GLM.

Discriminative Learning of GLM

- Generalized linear model (GLM):

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moderly called cross-entropy loss.

The Binary Case: A Detailed Look

- Binary classification, $y \in \{1, 0\}$, thus

$$f_{Y|\boldsymbol{X}}(1|\boldsymbol{x}) = \frac{\exp\left((\boldsymbol{\eta}^{(1)})^T\boldsymbol{\phi}(\boldsymbol{x}) + \zeta^{(1)}\right)}{\exp\left((\boldsymbol{\eta}^{(1)})^T\boldsymbol{\phi}(\boldsymbol{x}) + \zeta^{(1)}\right) + \exp\left((\boldsymbol{\eta}^{(0)})^T\boldsymbol{\phi}(\boldsymbol{x}) + \zeta^{(0)}\right)}$$

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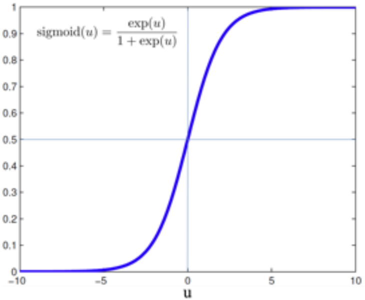

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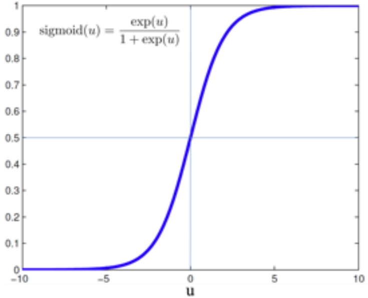

- Since $f_{Y|\boldsymbol{X}}(0|\boldsymbol{x}) = 1 - f_{Y|\boldsymbol{X}}(1|\boldsymbol{x})$,

$$f_{Y|\boldsymbol{X}}(0|\boldsymbol{x}) = \frac{1}{1+\exp\left(\boldsymbol{w}^T\boldsymbol{\phi}(\boldsymbol{x})\right)} = \frac{\exp\left(-\boldsymbol{w}^T\boldsymbol{\phi}(\boldsymbol{x})\right)}{1+\exp\left(-\boldsymbol{w}^T\boldsymbol{\phi}(\boldsymbol{x})\right)}$$

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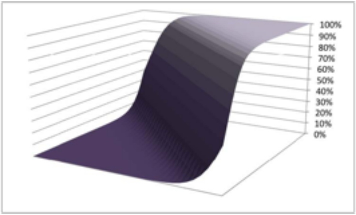
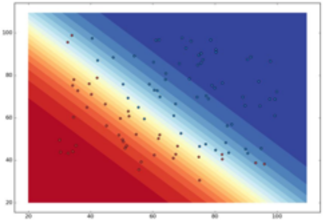
- In two dimensions $(\boldsymbol{w}, \boldsymbol{\phi}(\boldsymbol{x}) \in \mathbb{R}^2)$





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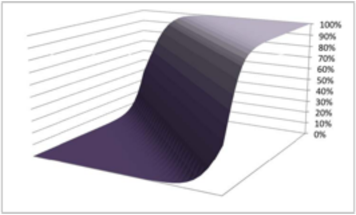

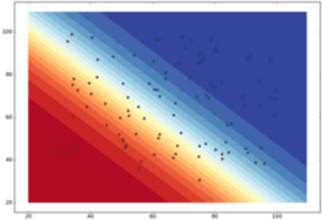

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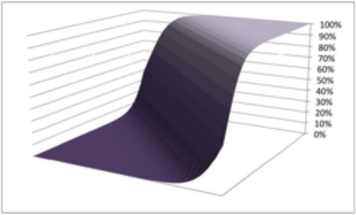

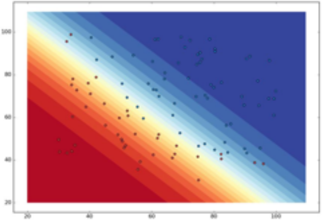

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- For any other threshold, $f_{Y|\boldsymbol{X}}(1|\boldsymbol{x}) = \tau \;\Leftrightarrow\; \boldsymbol{w}^T\boldsymbol{\phi}(\boldsymbol{x}) = \log(\frac{\tau}{1-\tau})$, is linear with respect to $\boldsymbol{\phi}(\boldsymbol{x})$.

Binary Logistic Regression: Log-Likelihood

- $f_Y(y|\boldsymbol{x}) = \left(\dfrac{\exp\left(\boldsymbol{w}^T\boldsymbol{\phi}(\boldsymbol{x})\right)}{1+\exp\left(\boldsymbol{w}^T\boldsymbol{\phi}(\boldsymbol{x})\right)}\right)^y \left(\dfrac{1}{1+\exp\left(\boldsymbol{w}^T\boldsymbol{\phi}(\boldsymbol{x})\right)}\right)^{(1-y)}$

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- $\mathcal{L}(\boldsymbol{w})$ is smooth and convex (should not be too hard to optimize)

Logistic Regression: the Separable Case

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- In this case, the ML parameter estimate is undefined.

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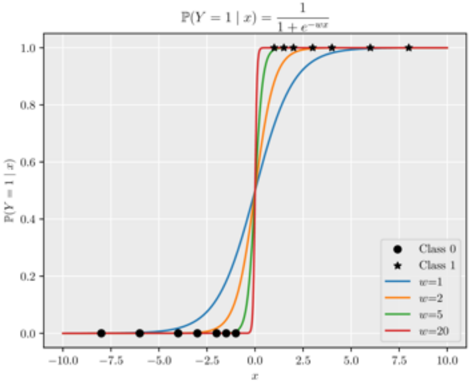
- For $y_i = 0$, $f_{Y|X}(0|x_i) = 1 - \text{sigmoid}(w\, x_i)$ also increases with w.



Ridge and LASSO Logistic Regression

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- Both well defined, even for separable data.

Multi-class Logistic Regression

- Recall the GLM, assuming, without loss of generality that $\phi(\boldsymbol{x}) = \boldsymbol{x}$ and $\zeta^{(y)} = 0$

$$f_{Y|\boldsymbol{X}}(y|\boldsymbol{x}, \boldsymbol{w}) = \frac{\exp\left(\boldsymbol{x}^T \boldsymbol{w}^{(y)}\right)}{\sum_{u=1}^{K} \exp\left(\boldsymbol{x}^T \boldsymbol{w}^{(u)}\right)}$$

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- The log-likelihood function can be written

$$\sum_{i=1}^{n} \log f_{Y|\boldsymbol{X}}(y_i|\boldsymbol{x}_i, \boldsymbol{w}) = \sum_{i=1}^{n} \sum_{k=1}^{K} \mathbf{1}_{y_i=k} \log f_{Y|\boldsymbol{X}}(k|\boldsymbol{x}_i, \boldsymbol{\eta}),$$

where $\mathbf{1}_{y_i=k} = 1$, if $y_i = k$, and $\mathbf{1}_{y_i=k} = 0$, if $y_i \neq k$.

Multi-class Logistic Regression (2)

- Using one-hot encoding: $\boldsymbol{y}_i \in \{0,1\}^K$, $y_{ik} = 1$ if $\boldsymbol{x}_i$ is in class k

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- Notice: if $\boldsymbol{x}_i$ is in class k, minimizing $\mathcal{L}(\boldsymbol{w})$ pushes $\boldsymbol{x}_i^T \boldsymbol{w}^{(k)}$ up.

Bayesian Logistic Regression

- Using some estimate $\hat{\boldsymbol{w}}$, obtained from data $\mathcal{D}$, and plugging it into $f_{Y|\boldsymbol{X}}(y|\boldsymbol{x},\hat{\boldsymbol{w}})$ ignores the randomness/uncertainty in $\hat{\boldsymbol{w}}$

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- Unfortunately, none of these have closed-form expressions.

Bayesian Logistic Regression (2)

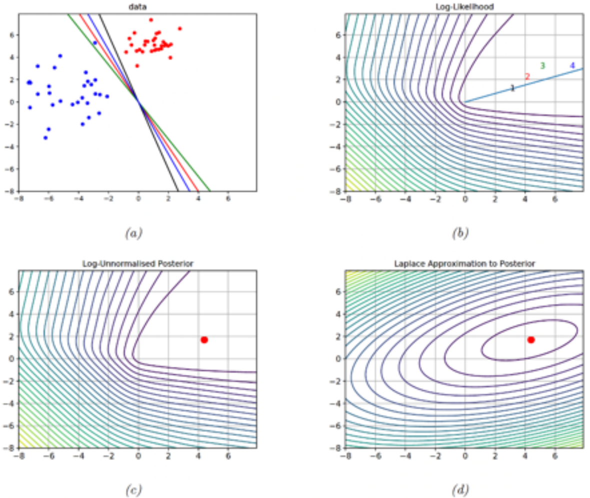


Figure 10.13: (a) Illustration of the data. (b) Log-likelihood for a logistic regression model. The line is drawn from the origin in the direction of the MLE (which is at infinity). The numbers correspond to 4 points in parameter space, corresponding to the lines in (a). (c) Unnormalized log posterior (assuming vague spherical prior). (d) Laplace approximation to posterior. Adapted from a figure by Mark Girolami. Generated by code at figures.probml.ai/book1/10.13.

Bayesian Logistic Regression (3)

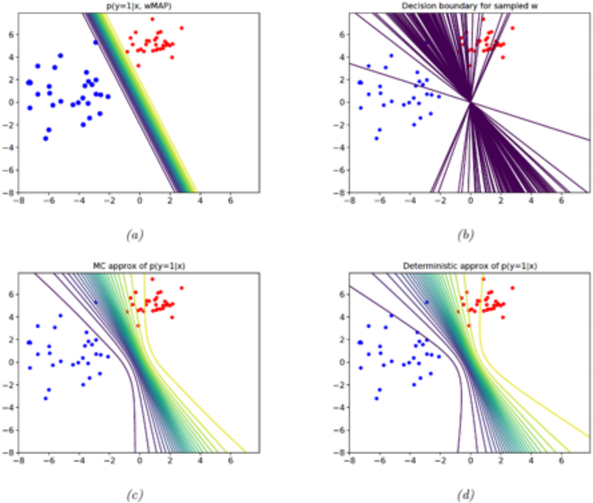
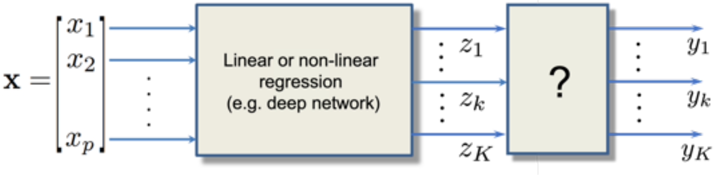


Figure 10.14: Posterior predictive distribution for a logistic regression model in 2d. (a): contours of $p(y=1|\boldsymbol{x}, \hat{\boldsymbol{w}}_{map})$. *(b): samples from the posterior predictive distribution. (c): Averaging over these samples. (d): moderated output (probit approximation). Adapted from a figure by Mark Girolami. Generated by code at* figures.probml.ai/book1/10.14.

Another View of (and Beyond) Softmax



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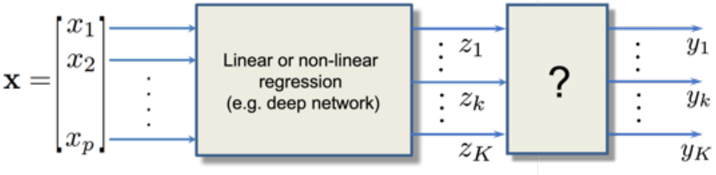

- Scores: $\boldsymbol{z} \in \mathbb{R}^K$, without constraints/restrictions.

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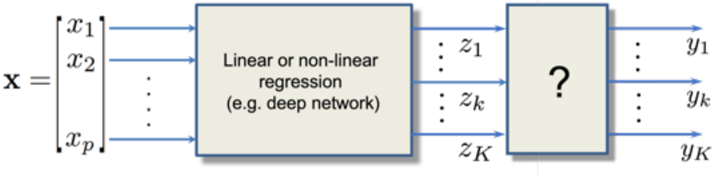

- Scores: $\boldsymbol{z} \in \mathbb{R}^K$, without constraints/restrictions.
- Probabilities: $y_k = \mathbb{P}[\text{class } k|\boldsymbol{x}]$, thus $\boldsymbol{y} \in \Delta_{K-1}$, where

$$\Delta_{K-1} = \left\{ \boldsymbol{y} \in \mathbb{R}^K, \text{ s.t. } y_1, ..., y_K \geq 0 \text{ and } \sum_{k=1}^{K} y_i = 1 \right\} \qquad \text{(simplex)}$$

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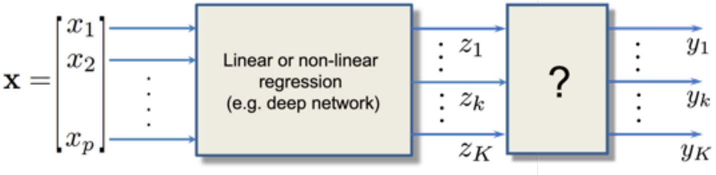

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- How to map from $\boldsymbol{z} \in \mathbb{R}^K$ to $\boldsymbol{y} \in \Delta_{K-1}$, such that

$$z_i = z_j \;\Rightarrow\; y_i = y_j \quad \text{and} \quad z_i > z_j \Rightarrow y_i \geq y_j$$

Argmax and Softmax

- First possibility: probability vector "most aligned" with $\boldsymbol{z}$:

$$\boldsymbol{y} = \arg \max_{\boldsymbol{p} \in \Delta_{K-1}} \boldsymbol{p}^T \boldsymbol{z} \quad \Longrightarrow \quad y_k \neq 0 \Leftrightarrow k \in \arg\max_j \{z_j,\ j = 1, ..., K\}$$

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- Second possibility: encourage more uniform probability distribution:

$$\boldsymbol{y} = \arg \max_{\boldsymbol{p} \in \Delta_{K-1}} \boldsymbol{p}^T \boldsymbol{z} + H(\boldsymbol{p})$$

where $H(\boldsymbol{p})$ is Shannon's entropy,

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- H satisfies: $H(\boldsymbol{p}) \geq 0$ and $H(\boldsymbol{p}) \leq \log K$ (attained for $p_i = 1/K$).

Softmax as Maximum Entropy

- Encouraging high entropy (with weight $1/\beta$):

$$\boldsymbol{y} = \arg \max_{\boldsymbol{p} \in \Delta_{K-1}} \beta\, \boldsymbol{p}^T \boldsymbol{z} \; + \; H(\boldsymbol{p})$$

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- Choosing λ to satisfy the constraint $\mathbf{1}^T \boldsymbol{p} = 1$ determines $Z(\beta, \lambda)$

$$y_i = \frac{e^{\beta\, z_i}}{\sum_{j=1}^K e^{\beta\, z_j}} = \big[\mathbf{softmax}(\beta\, \boldsymbol{z})\big]_i$$

Beyond Softmax: Sparsemax

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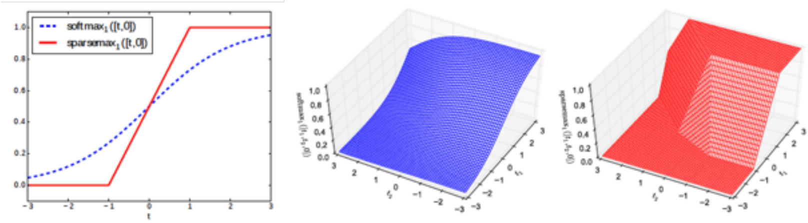
- Sparsemax versus softmax:



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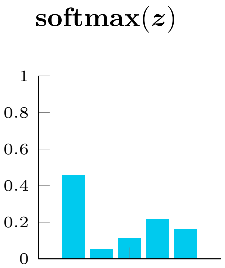
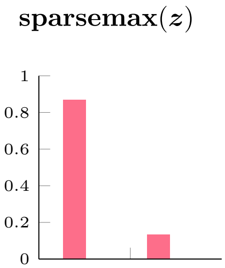
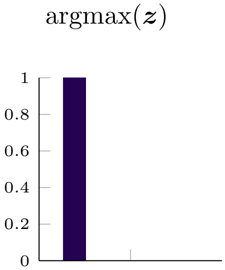
- For $\boldsymbol{z} = [1.0716, -1.1221, -0.3288, 0.3368, 0.0425]$







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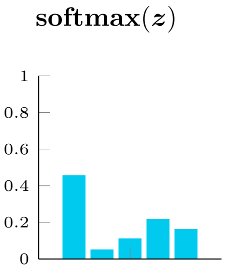

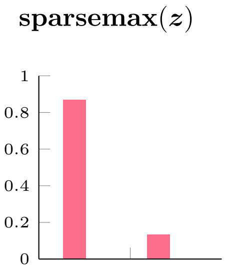

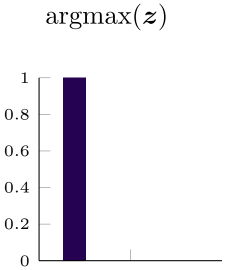

- Sparsemax, unlike softmax, may yield exact zeros.

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- The temperature controls how peaked the softmax is and how sparse the sparsemax is.

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  ... underlies support vector machines (SVM)

Classification: The Loss Function Perspective (2)

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$$L_{\text{error}}(f, y) \propto \mathbf{1}_{y\,f<0} = \begin{cases} 1 & \Leftarrow \quad \text{sign}(f) \neq y \\ 0 & \Leftarrow \quad \text{sign}(f) = y \end{cases}$$

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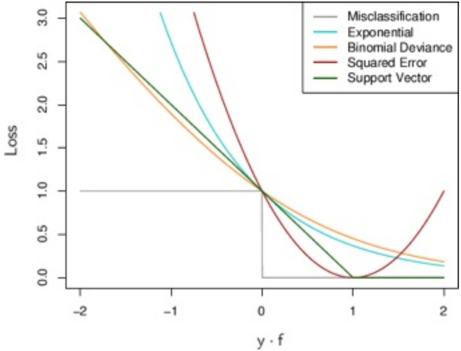

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- Not directly applicable to sparsemax: cannot compute $\log(0)$

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- This is achieved with the sparsemax loss:

$$\mathcal{L}(\boldsymbol{W}; (\boldsymbol{x}, \boldsymbol{y})) = -z_y(\boldsymbol{x}) + \frac{1}{2} \| \textbf{sparsemax}(\boldsymbol{z}(\boldsymbol{x})) \|^2 - \boldsymbol{z}(\boldsymbol{x})^\top \textbf{sparsemax}(\boldsymbol{z}(\boldsymbol{x})),$$

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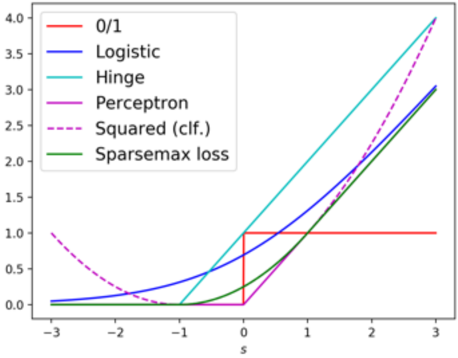
Classification Losses (Binary Case)

- Let the true label be $y = 1$ and define $s = z_2 - z_1$.
- Sparsemax loss is sort of a "classification Huber loss":



Outline

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- Hinge loss: $L_{\text{hinge}}(f, y) \propto \max\{0, 1 - y\, f\}$
- Absolute error loss: $L_{\text{abs}}(f, y) \propto |f - y|$ (not covered today)

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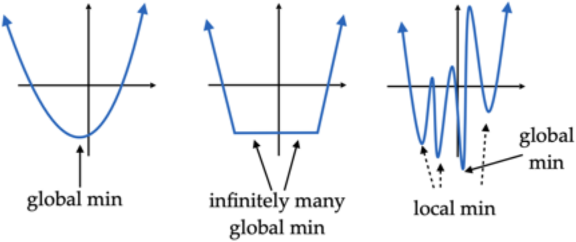
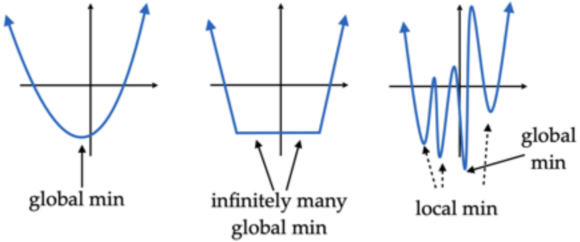
  - ✓ local, if $F(\boldsymbol{\theta}^*) \leq F(\boldsymbol{\theta})$, for any $\boldsymbol{\theta} \in \mathbb{R}^d$ s.t. $\|\boldsymbol{\theta} - \boldsymbol{\theta}\| \leq \varepsilon$, for some ε.



Minimizers

- Goal: find $\boldsymbol{\theta}^*$, a minimizer of $F(\boldsymbol{\theta})$ with respect to $\boldsymbol{\theta} \in \mathbb{R}^d$
- Types of minimizers:
  - ✓ global, if $F(\boldsymbol{\theta}^*) \leq F(\boldsymbol{\theta})$, for any $\boldsymbol{\theta} \in \mathbb{R}^d$
  - ✓ local, if $F(\boldsymbol{\theta}^*) \leq F(\boldsymbol{\theta})$, for any $\boldsymbol{\theta} \in \mathbb{R}^d$ s.t. $\|\boldsymbol{\theta} - \boldsymbol{\theta}\| \leq \varepsilon$, for some ε.



- Minimizers: global $\Rightarrow$ local; local $\not\Rightarrow$ global.

Convexity

- F is a convex function if, for all $\boldsymbol{\theta}_1,\, \boldsymbol{\theta}_2 \in \mathbb{R}^d$,

$$\lambda \in [0,\, 1] \;\Rightarrow\; F(\lambda\boldsymbol{\theta}_1 + (1-\lambda)\boldsymbol{\theta}_2) \leq \lambda F(\boldsymbol{\theta}_1) + (1-\lambda)F(\boldsymbol{\theta}_2)$$

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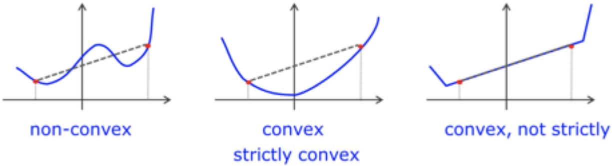

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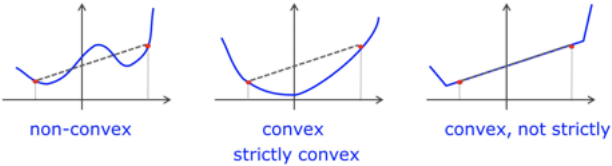

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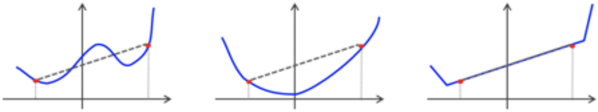

non-convex

convex
strictly convex

convex, not strictly

- Convexity $\Rightarrow$ all local minima are global minima.

- Convexity $\Rightarrow$ continuity.

Hessian

- For F twice differentiable, the Hessian is

$$H(\boldsymbol{\theta}) = \nabla^2 F(\boldsymbol{\theta}) = \begin{bmatrix} \frac{\partial^2 F}{\partial \theta_1^2} & \frac{\partial^2 F}{\partial \theta_1 \partial \theta_2} & \cdots & \frac{\partial^2 F}{\partial \theta_1 \partial \theta_d} \\ \frac{\partial^2 F}{\partial \theta_2 \partial \theta_1} & \frac{\partial^2 F}{\partial \theta_2^2} & \cdots & \frac{\partial^2 F}{\partial \theta_2 \partial \theta_d} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 F}{\partial \theta_d \partial \theta_1} & \frac{\partial^2 F}{\partial \theta_d \partial \theta_2} & \cdots & \frac{\partial^2 F}{\partial \theta_d^2} \end{bmatrix} \in \mathbb{R}^{d \times d}$$

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- F strictly convex $\Leftrightarrow$ $H(\boldsymbol{\theta}) \succ 0$ (positive definite — pd)

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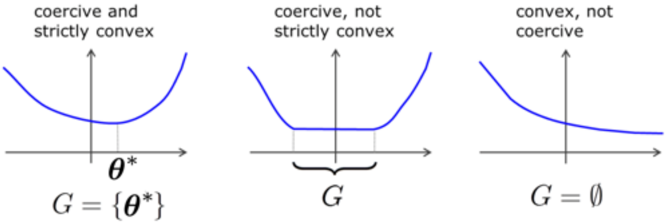

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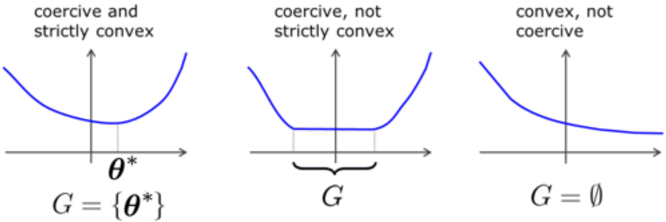

- Non-coercivity example: logistic regression on separable data.

Descent Directions

- Definition: $\boldsymbol{\eta}$ is a descent direction at $\boldsymbol{\theta}_0$ if

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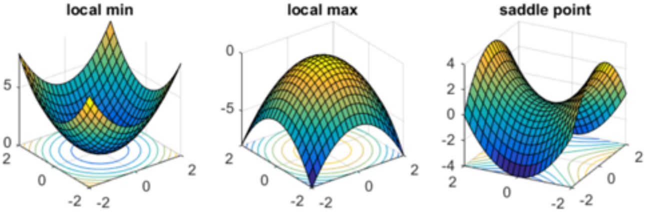

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- Can also be proved without the Hessian (see recommended reading).

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- If $\mathbf{X}$ is full (column) rank, then $\mathbf{Q} \succ 0$, thus F is strictly convex (unique minimizer).

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- Convergence requires unique $\boldsymbol{\theta}^*$, thus $\mathbf{Q} \succ 0$, *i.e.*, $\lambda_{\text{min}}(\mathbf{Q}) > 0$.

Gradient Descent: Quadratic Case (3)

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- Finally, $$\|\boldsymbol{\theta}_t - \boldsymbol{\theta}^*\|_2 \leq \left(\frac{\kappa - 1}{\kappa}\right)^t \|\boldsymbol{\theta}_0 - \boldsymbol{\theta}^*\|_2 \xrightarrow[t\to\infty]{} 0.$$

Gradient Descent: Quadratic Case (4)

- If $\lambda_{\text{min}}(\mathbf{Q})$ is known, there is a (slightly) better choice:

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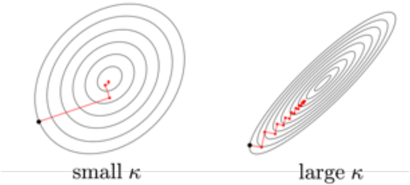
- This type of convergence is called linear:

$$\frac{\|\boldsymbol{\theta}_t - \boldsymbol{\theta}^*\|_2}{\|\boldsymbol{\theta}_{t-1} - \boldsymbol{\theta}^*\|_2} \leq \gamma < 1.$$

Gradient Descent: Quadratic Case (5)

- The condition number κ expresses the problem difficulty.



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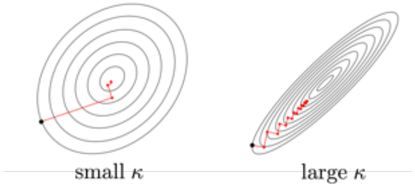
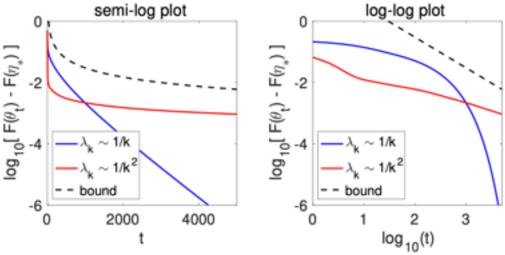


- Convergence for different distributions of eigenvalues.



(pictures from F. Bach).

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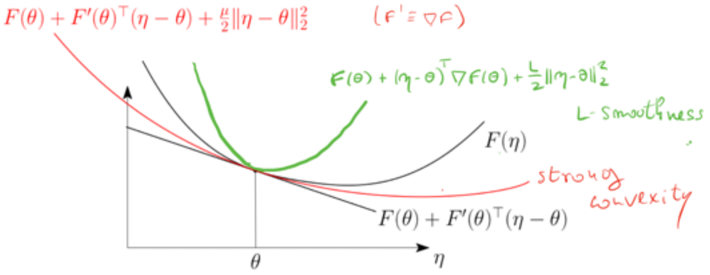
- L-smooth and $\mu-$strongly convex function: upper and lower bounded by quadratics.



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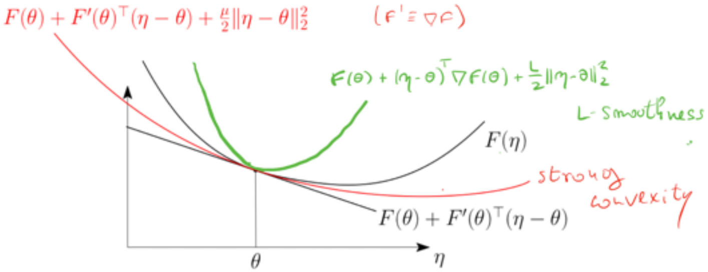

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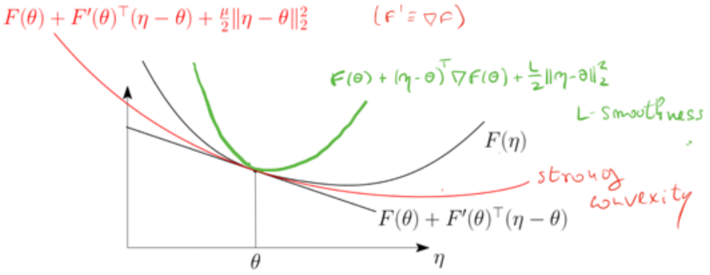

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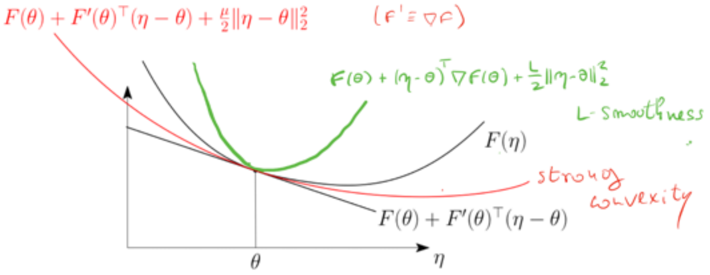

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- Regularization: if $F(\boldsymbol{\theta})$ is convex, $F(\boldsymbol{\theta}) + \frac{\mu}{2}\|\boldsymbol{\theta}\|_2^2$ is μ-strongly convex.

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- Gradient descent with step-size $\alpha = 1/L$,

$$F(\boldsymbol{\theta}_t) - F(\boldsymbol{\theta}^*) \leq \left(\frac{\kappa - 1}{\kappa}\right)^t \big(F(\boldsymbol{\theta}_0) - F(\boldsymbol{\theta}^*)\big)$$

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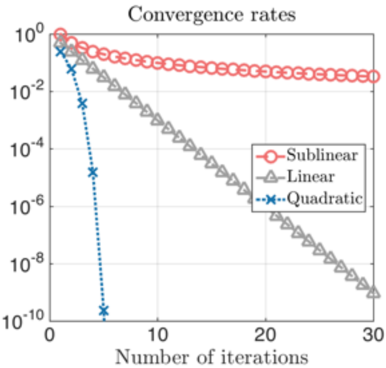
- Proofs: see recommended reading (F. Bach).

Linear vs Sublinear Convergence



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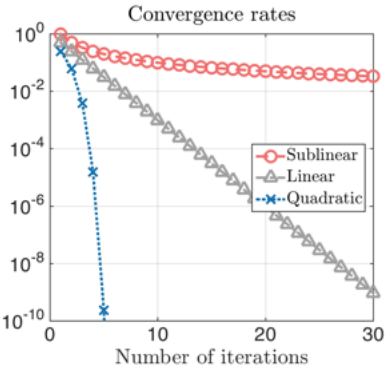

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- Back to empirical risk minimization: $\hat{\boldsymbol{\theta}} = \arg\min_{\boldsymbol{\theta}} F(\boldsymbol{\theta})$

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- Alternative: stochastic gradient "descent" (SGD):
  - ✓ Start at some initial point $\boldsymbol{\theta}_0 \in \mathbb{R}^d$
  - ✓ For $t = 1, 2, ...,$
    - ▷ sample $i \in \{1, ..., n\}$ at random and choose step-size α_t,
    - ▷ take a step of size α_t in the direction of the negative gradient:

$$\boldsymbol{\theta}_t = \boldsymbol{\theta}_{t-1} - \alpha_t \nabla L(f(\boldsymbol{x}_i;\boldsymbol{\theta}_{t-1}), y_i)$$

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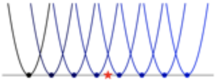

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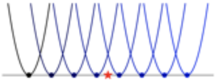

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Motivation for SGD: Computing a Mean

- Consider the goal of computing a mean: $\boldsymbol{\mu} = \frac{1}{n}\sum_{i=1}^{n} \boldsymbol{x}_i$.
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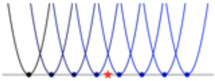

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- Notice that $(t-1)\boldsymbol{\theta}_{t-1} = \sum_{i=1}^{t-1} \boldsymbol{x}_i$, thus $\boldsymbol{\theta}_t = \frac{1}{t}\sum_{i=1}^{t} \boldsymbol{x}_i$

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- Goal: computing an expectation,

$$\mu = \mathbb{E}[X] = \arg\min_w \overbrace{\frac{1}{2}\,\mathbb{E}[(w - X)^2]}^{R(w)}$$

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- In expectation, SGD by sampling $f_{\boldsymbol{X},Y}$ is gradient descent on $\mathcal{R}(\boldsymbol{\theta})$.

Convergence of Stochastic Gradient Descent

- SGD uses noisy gradients: $\boldsymbol{G}(\boldsymbol{\theta})$, such that $\mathbb{E}[\boldsymbol{G}(\boldsymbol{\theta})] = \nabla F(\boldsymbol{\theta})$
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- Notice: not practical to compute $F(\boldsymbol{\theta}_t)$. Selecting the best iterate is thus impractical and would beat the purpose of SGD.

Convergence of SGD: Strongly Convex Case

- Regularization: $F(\boldsymbol{\theta}) = \dfrac{1}{n}\displaystyle\sum_{i=1}^{n} L(f(\boldsymbol{x}_i;\boldsymbol{\theta}), y_i) + \frac{\mu}{2}\|\boldsymbol{\theta}\|_2^2$

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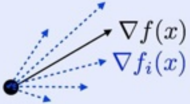
- Strong convexity speeds up convergence from $O(1/\sqrt{t})$ to $O(1/t)$

Visual Summary

Finite sums

$$f(x) \stackrel{\text{def.}}{=} \frac{1}{n}\sum_{i=1}^{n} f_i(x)$$
$$\nabla f(x) = \frac{1}{n}\sum_i \nabla f_i(x)$$

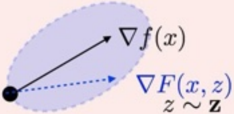


Draw $i \in \{1, \ldots, n\}$ uniformly.

$$x_{k+1} = x_k - \tau_k \nabla f_i(x_k)$$

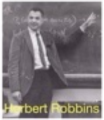
Expectation

$$f(x) \stackrel{\text{def.}}{=} \mathbb{E}_{\mathbf{z}}(f(x, \mathbf{z}))$$
$$\nabla f(x) = \mathbb{E}_{\mathbf{z}}(\nabla F(x, \mathbf{z}))$$



Draw $z \sim \mathbf{z}$

$$x_{k+1} = x_k - \tau_k \nabla F(x, z)$$



Theorem: If f is strongly convex and $\tau_k \sim 1/k$,

$$\mathbb{E}(\|x_k - x^\star\|^2) = O(1/k)$$

(Picture by Gabriel Peyré)

Stochastic Gradient Descent: Linear Classification

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showing that $\nabla \ell(y_i \boldsymbol{\theta}^T \boldsymbol{x}_i)$ is co-linear with $\boldsymbol{x}_i$.

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- Each SGD update moves $\boldsymbol{\theta}_t$ in a direction parallel to sample $\boldsymbol{x}_i$.

The Perceptron Algorithm

- Hinge loss: $\ell(u) = \max\{0, 1 - \tau\}$, thus

$$\frac{d\,\ell(u)}{d\,u} = \begin{cases} -1, & \text{if } u \leq \tau \\ 0, & \text{otherwise.} \end{cases}$$

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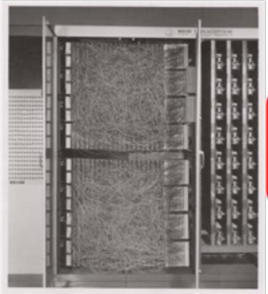
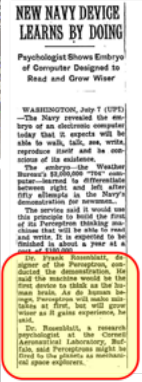
- This is the famous Perceptron algorithm, proposed in 1957 by Frank Rosenblatt (with $\tau = 0$), the percursor of modern neural networks.

A Bit of History: The Perceptron





NEW NAVY DEVICE LEARNS BY DOING

Psychologist Shows Embryo of Computer Designed to Read and Grow Wiser

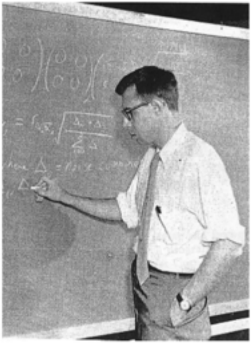
WASHINGTON, July 7 (UPI) —The Navy revealed the embryo of an electronic computer today that it expects will be able to walk, talk, see, write, reproduce itself and be conscious of its existence.

The embryo—the Weather Bureau's $2,000,000 "704" computer—learned to differentiate between right and left after fifty attempts in the Navy's demonstration for newsmen.

The service said it would use this principle to build the first of its Perceptron thinking machines that will be able to read and write. It is expected to be finished in about a year at a cost of $100,000.

Dr. Frank Rosenblatt, designer of the Perceptron, conducted the demonstration. He said the machine would be the first device to think as the human brain. As do human beings, Perceptron will make mistakes at first, but will grow wiser as it gains experience, he said.

Dr. Rosenblatt, a research psychologist at the Cornell Aeronautical Laboratory, Buffalo, said Perceptrons might be fired to the planets as mechanical space explorers.



The New York Times, 1958

Minsky and Pappert, 1969

Perceptron Mistake Bound

- Definitions:
  - ✓ The training data is linearly separable with margin $\gamma > 0$ iff there is a weight vector $\boldsymbol{u}$, with $\|\boldsymbol{u}\| = 1$, such that

$$y_n \, \boldsymbol{u}^T \boldsymbol{x}_n \geq \gamma, \quad \forall n.$$

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  - ✓ Radius of the data: $R = \max_n \|\boldsymbol{x}_n\|$.
- Then, the following bound of the number of mistakes holds[2]

Theorem

The perceptron algorithm is guaranteed to find a separating hyperplane after at most $\frac{R^2}{\gamma^2}$ *mistakes (non-zero updates).*

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Novikoff's Theorem: One-Slide Proof

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- Equating both sides, $(M\gamma)^2 \leq \|\boldsymbol{\theta}_t\|^2 \leq M\, R^2 \;\Rightarrow\; M \leq R^2/\gamma^2$ ■

Implicit Regularization

- SGD in linear prediction, with i_t denoting the sample at iteration t,

$$\boldsymbol{\theta}_t = \boldsymbol{\theta}_{t-1} - \alpha_t \, e_{i_t} \, \boldsymbol{x}_{i_t}$$

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- If there are multiple $\boldsymbol{\theta}^*$ with $F(\boldsymbol{\theta}^*) = 0$, and the predictions only depend on $\boldsymbol{\theta}^T \boldsymbol{x}_i$, this corresponds to solving

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- This is sometimes called the overparametrized or interpolating regime and is a central tool in the understanding of modern deep learning.

Explicit Regularization: Weight Decay

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- $\boldsymbol{\theta}_{t-1}$ is shrunk/decayed before being updated: weight decay

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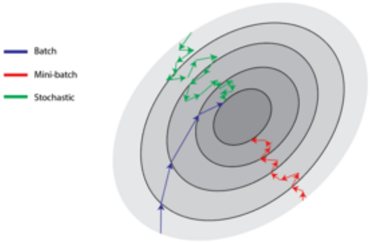
- Minibatching: instead of a single sample, use minibatches (size m)

$$\boldsymbol{\theta}_t = \boldsymbol{\theta}_{t-1} - \frac{\alpha_t}{m} \sum_{j \in \text{minibatch } t} \nabla L(f(\boldsymbol{x}_j; \boldsymbol{\theta}_{t-1}), y_j)$$



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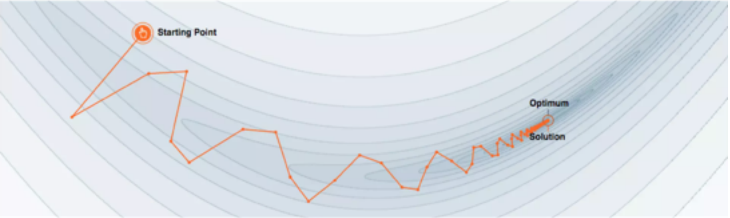
- Advantage: reduces the update in directions with changing gradients; increases the update in directions with stable gradient.



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- Advantages: Computationally efficient, low memory usage, suitable for large datasets and many parameters.
- Drawbacks: Possible convergence issues and noisy gradient estimates.

[5] D. Kingma, J. Ba, "Adam: A Method for Stochastic Optimization", *International Conference for Learning Representations*, 2015. (more than 184000 citations)

Conclusions

Conclusions

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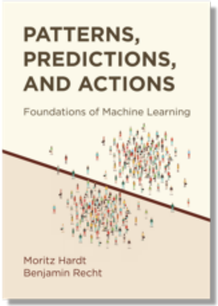
Let's have lunch!!

Recommended Books



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Learning Theory from First Principles

June 8, 2024

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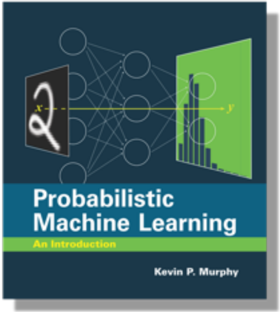
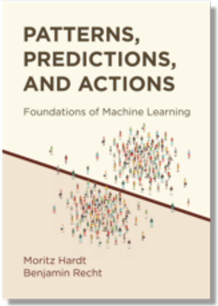
https://www.di.ens.fr/~fbach/ltfp_book.pdf



https://probml.github.io/pml-book/book1.html

Recommended Books



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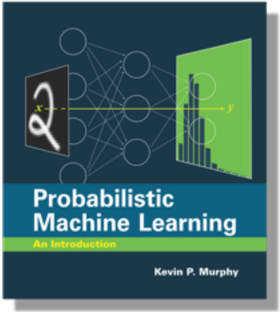

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Thank you! Questions?